

Comment on “Floquet spin states in graphene under ac-driven spin-orbit interaction”

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Recently, López *et al.*¹ applied the Magnus-Floquet expansion² (MFE) to the quasi-energy spectrum and the related dynamical features in monolayer graphene under the periodically Rashba spin-orbit interaction. They suggested this approach to be an efficient tool to deal with time-dependent problems and further claimed that the results from this approach converge faster than those from the standard Floquet-Fourier approach^{3–8} for a weak field strength. In the following, we will demonstrate that many results in that paper are in fact beyond the convergence domain of the MFE and hence are incorrect.

We first plot the quasi-energies of the lowest conduction-like Floquet band ϵ_+ , taken from Fig. 1 in Ref. 1, as blue squares in Fig. 1(a). They are obtained via the MFE up to the third order:^{1,2}

$$\epsilon_+^{\text{up to (3)}} = \Omega \kappa \sqrt{16\kappa^2 \Lambda^2 + (\Lambda^2 - 1)^2}, \quad (1)$$

where $\kappa = v_F k / \Omega$ and $\Lambda = \lambda_R / \Omega$, with λ_R and Ω being the magnitude and frequency of the ac-driven Rashba spin-orbit coupling. Since the value of Λ was not given in that paper, we fit their results with Eq. (1). The best fitting gives $\Lambda = 1.25$, with the corresponding results plotted as blue dashed curve. It is seen that no quasi-energy gap opens in the whole momentum regime. This behavior is very much different from that in graphene irradiated by a laser field.^{5–8} However, the Hamiltonian in this system is similar to the latter one. This can be seen more clearly by transforming the Hamiltonian given by Eq. (11) in Ref. 1 into the basis set formed by the eigenvectors of its time-independent term. The Hamiltonian becomes

$$\tilde{h}_-(k, t) = v_F k \sigma_z - \lambda_R \cos \Omega t (I + \sigma_x), \quad (2)$$

with I and σ being the identity and Pauli matrices, respectively. By comparing this equation with Eqs. (B3) and (B4) in our work,⁷ one can find $\tilde{h}_-(k, t)$ shares the identical quasi-energy spectrum with that in graphene under a linearly polarized laser field with the momentum perpendicular to the direction of the laser field. In the latter case, the previous investigations^{6–8} have demonstrated that quasi-energy gaps appear at nonzero momentum [a typical case can be seen in Fig. 3(b) in Ref. 7]. This indicates that the quasi-energy spectrum reported by López *et al.*¹ are questionable.

We further calculate the corresponding quasi-energies of Eq. (2) from the Floquet-Fourier approach^{3–8} [red solid curve in Fig. 1(a)]. This approach transforms the solving of the time-dependent Schrödinger equation into an

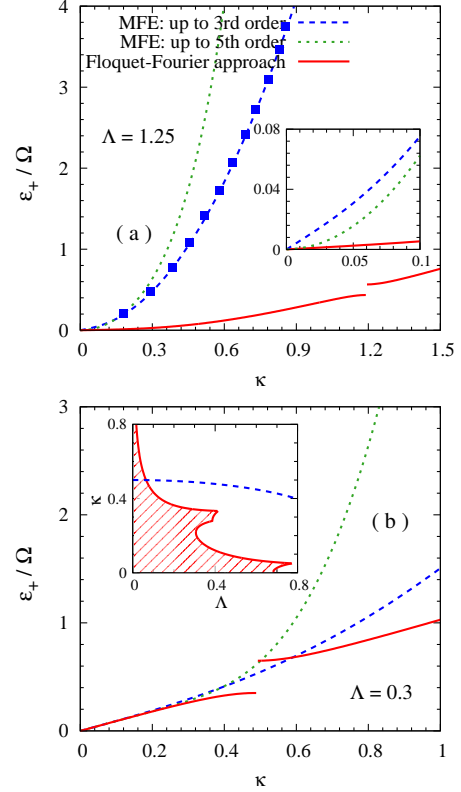


FIG. 1: (Color online) The quasi-energies ϵ_+ from the MFE up to third (blue dashed curves) and fifth (green dotted curves) orders as well as those from the Floquet-Fourier approach (red solid curves) for $\Lambda = 1.25$ (a) and 0.3 (b). The blue squares in (a) are taken from Fig. 1 in Ref. 1. The region for $\kappa < 0.1$ in (a) is enlarged in its inset. In the inset of (b), the convergence regime of the MFE (the shadow area) and the momentum corresponding to the first quasi-energy gap as function of Λ (blue dashed curve) are plotted.

eigenvalue problem of the Hamiltonian in the Fourier basis set. By increasing the number of the Fourier mode, one can obtain the quasi-energy and eigenstates with any degree of accuracy in principle. Here we calculate the quasi-energies of the system in Ref. 1 via this approach using 30 Fourier modes. The relative error are verified to be smaller than 10^{-5} . From Fig. 1(a), one observes that the results from the MFE are *qualitatively* different from the exact results from the Floquet-Fourier approach. In particular, a gap appears in the quasi-energy spectrum from the Floquet-Fourier approach, in agreement with

the analysis of the Hamiltonian, but is absent in those from MFE. This comparison further confirms that the quasi-energy spectrum in that paper is incorrect. In addition, the results in Figs. 4 and 6 in that paper are based on the same approach with the same parameter, and hence are questionable as well.

In order to reveal the reason leading to this problem, we plot the quasi-energies from the MFE up to the fifth order as green dotted curve. The corresponding formula reads^{1,2,9}

$$\begin{aligned} \varepsilon_+^{\text{up to (5)}} &= \frac{\Omega\kappa}{36} [331776\kappa^6\Lambda^2 - 2304\kappa^4(23\Lambda^4 - 72\Lambda^2) \\ &+ 32\kappa^2(1109\Lambda^6 - 900\Lambda^4 - 324\Lambda^2) + 81(\Lambda^2 - 2)^4]^{\frac{1}{2}}. \end{aligned} \quad (3)$$

One observes that the difference between the results from the MFE up to the third and fifth orders is considerably grave even at small momentum (the region for $\kappa < 0.1$ is enlarged in the inset). Further calculations show that the convergence criterion, chosen to be $|\varepsilon_+^{\text{up to (5)}} - \varepsilon_+^{\text{up to (3)}}|/\varepsilon_+^{\text{up to (3)}} < 10\%$ and $|\partial_\kappa \varepsilon_+^{\text{up to (5)}} - \partial_\kappa \varepsilon_+^{\text{up to (3)}}|/\partial_\kappa \varepsilon_+^{\text{up to (3)}} < 10\%$ here, cannot be satisfied in the whole momentum regime. This indicates that the discrepancy between the quasi-energies from the MFE and the Floquet-Fourier approach is due to the fact that the results from the MFE do not converge.

We also plot the quasi-energies ε_+ from the above ap-

proaches for a weaker field strength $\Lambda = 0.3$ in Fig. 1(b). It is seen that ε_+ from Eq. (1) agrees well with the exact one from the Floquet-Fourier approach in the convergence regime of the MFE, but deviates markedly beyond the convergence regime, e.g., at the momentum corresponding to the quasi-energy gap. This agrees with the discussions presented above. We further plot the convergence regime of the MFE as well as the momentum corresponding to the first quasi-energy gap as function of Λ in the inset of Fig. 1(b). From this inset, one finds that the approach of the MFE only converges for small momentum and weak ac field. Moreover, the parameter used in Ref. 1, i.e., $\Lambda = 1.25$, is well beyond the convergence regime which is in consistence with the results shown in Fig. 1(a). It is also shown that except for extremely small Λ , where the exact quasi-energy spectrum is very close to the field-free one (the relative difference is smaller than 10%) and the quasi-energy gap is still negligible, the maximum momentum of the convergence regime is always smaller than the momentum corresponding to the first quasi-energy gap. This explains why the results from the MFE cannot reproduce the gap-like behavior.

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⁹ Here we have corrected the error in Eq. (A9) in Ref. 1. In addition, Eq. (A6) in that paper should be corrected as $F_1 = i\kappa(\kappa\sigma_z + \Lambda\sigma_x)/\sqrt{\kappa^2 + \Lambda^2}$.